Learning Gibbs-regularized GANs with variational discriminator reparameterization

Abstract

We propose a novel approach to regularizing generative adversarial networks (GANs) leveraging learned *structured Gibbs distributions*. Our method consists of reparameterizing the discriminator to be an explicit function of two densities: the generator PDF q and a structured Gibbs distribution ν. Leveraging recent work on invertible pushforward density estimators, this reparameterization is made possible by assuming the generator is invertible, which enables the analytic evaluation of the generator PDF q. We further propose optimizing the Jeffrey divergence, which balances mode coverage with sample quality. The combination of this loss and reparameterization allows us to effectively regularize the generator by imposing structure from domain knowledge on ν, as in classical graphical models. Applying our method to a vehicle trajectory forecasting task, we observe that we are able to obtain quantitatively superior mode coverage as well as better-quality samples compared to traditional methods.

1 Introduction

Although high-dimensional generative modeling has made significant advances recently with the advent of GANs and related methods, one may argue that these recent methods have taken a step back in one significant respect: regularization. Classical generative models based on graphical models addressed this issue mainly by imposing some kind of structure directly on the joint distribution— e.g., by assuming that the joint distribution factorizes into a product of sparsely connected cliques. Although this is a flexible framework admitting the imposition of many different kinds of domain knowledge as regularization, the trade-off is that inference in graphical models is generally intractable.

GANs select the opposite trade-off: we can efficiently sample a GAN, but regularization is difficult, as we cannot impose structure directly on the joint distribution of a GAN's outputs. We submit that regularizing the structure of a GAN's generator and discriminator is generally more difficult than imposing meaningful structure directly on the model distribution, which we will refer to as $q : \mathbb{R}^N \to \mathbb{R}^+$. First, observe that the generator $f : \mathbb{R}^D \to \mathbb{R}^N$ is intrinsically more complex entity than q—it must *produce* a high-dimensional output from a potentially high-dimensional input, whereas q need only produce a *scalar summary* of a high-dimensional input. Second, while we can borrow from the graphical models literature to structure q in an appropriate way for many different domains, a generator is comparatively harder to regularize using domain knowledge because it is effectively a causal model of generation—one that usually bears no resemblance to the *true* generation process, which is most often unobserved or exceedingly difficult to model. Consider image generation: although it is plausible—e.g., from biological arguments—that convolutional neural networks constitute a good class of image classifiers, claiming CNNs are inherently well-suited to image *generation* is harder to justify. Even in the exceptional case that we can regularize the structure of a generator in a plausible way using domain knowledge, we are still left with no guidance as to how to regularize the structure of the *discriminator*; although recent methods have seen some success in applying generic smoothness regularizers to the discriminator [3, 13, 37], it is not obvious how to impose *domain-specific* structure on the discriminator in an optimal way.

As a remedy to this situation, we propose shifting the burden of regularization largely onto the discriminator and reparameterizing the discriminator, representing it as a function of the generator density q and a *structured Gibbs distribution* ν that directly approximates the target density p. Doing so allows us to directly impose known regularities from the target domain on ν—just as in classical

Figure 1: Top: Illustration of alternating optimization of Eq. (1). $\widetilde{KL}_\nu(q, p)$ denotes variational approximation of $KL(q, p)$ with variational parameters ν. **Bottom:** Our method applied to forecast ego-vehicle trajectories, showing input image and overhead views with the learned cost $-\log(\nu)$ (overlaid on LIDAR map). Middle shows samples from current q (red), and true future path (cyan). Note that ν has learned to penalize regions with obstacles ($V(x) = \log \nu(x)$, *i.e.* higher $V(x)$ is lower traversal cost). Right: after incorporating the learned ν, q and its samples are shifted to avoid high-cost regions, corresponding to suppression of spurious modes (as in chart D).

unnormalized graphical models, such as CRFs [21] and EBMs [22]. These regularities can consist of symmetries, invariances, and/or graphical model structure: for example, we may assume that $\log \nu$ is written as a sum of local clique potentials for a problem with temporal or spatial structure; for an image-generation problem, $\log \nu$ may reasonably take the form of a CNN, if we believe that the target density p should be approximately translation-invariant.

This reparameterization may be obtained by appealing to the f-GAN formulation [29], which interprets and generalizes the typical GAN objective from a variational perspective. This perspective reveals the optimal discriminator T to be a function of the odds ratio: $T^* = h(q/p)$, for some function h determined by the particular f-divergence chosen. We observe that if q can be evaluated, then we can reparameterize the discriminator as $T = h(q/\nu)$, where ν directly approximates the target density p. By imposing known regularities of p on ν, we can effectively regularize the discriminator using domain knowledge, as described above. Note that we cannot naively impose the same structure on T, because T may not have that structure: if we think of p as a function in a class A, and q as a function in a class B, it is clear that $T = h(q/p)$ will generally not be in either A or B. Fig. 1 illustrates how ν is structured for our application domain of vehicle trajectory forecasting: ν is represented as a sum of learned spatial rewards, which penalizes trajectories according to a learned function over spatial positions. Intuitively, this prevents trajectories from colliding with obstacles, while simultaneously learning the concept of an obstacle.

Another key observation that makes our proposal feasible is that q can be evaluated if the generator is invertible and differentiable [32, 9, 20]: in this case, q (the *pushforward* density [7] of a simple density q_0 under the generator g) satisfies $q(g(z)) = q_0(z) |\det \frac{dg}{dz}|^{-1}$. Finally, we advocate training the model to minimize the symmetric KL (*Jeffrey*) divergence $KL(p \parallel q) + KL(q \parallel p)$. Doing so allows us to start from a baseline model, $\min_q KL(p \parallel q)$, that can be pretrained without adversarial training and that additionally tends not to overfit [16, 6], even if q is induced by a very complex generator. Regularization of the model is then controlled largely by the subsequently added $KL(q \parallel p)$ term: we view this term as selectively pruning modes of q not supported by p. Regularizing ν using domain-specific structure prevents the pruning of modes similar to training examples under the invariances built into ν, as illustrated in Fig. 2.

2 APPROACH

Concretely, our method optimizes the following variational bound of $KL(p \parallel q) + KL(q \parallel p)$, which can be derived by applying the f-GAN formulation to $KL(q \parallel p)$ and applying the discriminator reparameterization $T = -q/\nu$:

$$\min_{q \in \mathcal{Q}} \sup_{\nu > 0} \mathbb{E}_{\hat{x} \sim p} \log \frac{p(\hat{x})}{q(\hat{x})} + \sup_{\nu > 0} -\mathbb{E}_{\hat{x} \sim p} \frac{q(\hat{x})}{\nu(\hat{x})} + \mathbb{E}_{x \sim q} \log \frac{q(x)}{\nu(x)}. \quad (1)$$

We first give intuition for Eq. (1) and discuss practical optimization aspects. We then derive and analyze the method from different perspectives to further elucidate the nature of the method.

Figure 1 illustrates how the method works in a hypothetical one-dimensional example. Chart *A* depicts the probability density function p of the data we wish to model. We cannot evaluate this function, but we can sample the distribution: locations of samples are marked by stars. Chart B depicts a model density q minimizing just the first part of our objective, $KL(p \parallel q)$. Unfortunately, since $KL(p \parallel q)$ is not sensitive to spurious modes in q, this may result in q having false modes [6]. Our solution is illustrated in charts C and D. We add an approximation of $KL(q \parallel p)$ to the objective, which heavily penalizes false modes in q. Since evaluating $KL(q \parallel p)$ requires the evaluation of the unknown density p, we learn another density ν that approximates p. The learning rule for ν is shown in the third chart: ν is implicitly pushed towards p at samples from q, until ν is a good approximation to p in the vicinity of samples from q. Finally, q is readjusted; in addition to raising the density of q at samples from p, the objective term $-\mathbb{E}_{x \sim q} \log \nu(x)$ sharply lowers the density of q wherever ν's density is low, effectively pruning false modes.

Intuition for the learning rule of ν can be obtained by computing the *functional gradient* of Eq. (1) with respect to ν (i.e., differentiating with respect to $\nu(x)$, $\forall x$). The functional gradient $\delta/\delta\nu$ expresses the direction in which ν should be moved at each point x in order to optimally decrease the objective. Observing that $E_{x \sim p} q(x)/\nu(x) = E_{x \sim q} p(x)/\nu(x)$, we obtain the following for the functional gradient of the objective wrt. $\log \nu$: $\delta C/\delta \log \nu(x) = q(x)\left(p(x)/\nu(x) - 1\right)$. We therefore see that minimizing Eq. (1) in ν raises or lowers $\log \nu$ at each point x according to whether it exceeds $p(x)$, with a learning rate given by $q(x)$, and a unique fixed point (assuming $q > 0$) of $p = \nu$. See chart C.

2.1 PUSHFORWARD REPRESENTATION OF q

Optimizing Eq. (1) is straightforward except for one subtle point: we must be able to evaluate q pointwise and differentiate the expression $\mathbb{E}_{x \sim q} \log(q(x)/\nu(x))$ with respect to the parameters of q. Inspired by prior work [32, 9, 20], we solve both these problems by representing q as the *pushforward* of a simple distribution under an invertible warp (also known as a normalizing flow). Suppose μ is a distribution over a set Z and $g : Z \to X$ is a function (the *generator*) with domain Z. Then we can define a measure on X as the distribution of $g(z)$ sampling z from μ—this distribution, denoted here by $g|_{\mu}$, is referred to as the pushforward of μ under g.

Now suppose g is parameterized by θ and differentiable in x and θ. By representing q as $q_{\theta} = g_{\theta}|_{\mu}$, for some simple distribution μ, we can move the derivative wrt. θ inside the expectation by exploiting the property $\mathbb{E}_{x \sim g_{\theta}|_{\mu}} f(x) = \mathbb{E}_{z \sim \mu} f(g_{\theta}(z))$ for all functions f:

$$\frac{\mathrm{d}}{\mathrm{d}\theta} \mathbb{E}_{x \sim q} \log \frac{q(x)}{\nu(x)} = \frac{\mathrm{d}}{\mathrm{d}\theta} \mathbb{E}_{x \sim q_{\theta}|_{\mu}} \log \frac{q(x)}{\nu(x)} = \mathbb{E}_{x \sim \mu} \frac{\mathrm{d}}{\mathrm{d}\theta} \log \frac{q_{\theta}(g_{\theta}(x))}{\nu(g_{\theta}(x))}. \quad (2)$$

This is well-known as the *reparameterization trick*; it allows us to obtain a low-variance, unbiased estimate of the parameter derivatives for learning with SGD. However, one problem remains: evaluating $q_{\theta}(x) = (g_{\theta}|_{\mu})(x)$, which appears in both the first and last terms of (1). This is solved by assuming that g_{θ} is invertible: $\hat{z} := g_{\theta}^{-1}(\hat{x})$. Thus, we have an analytic formula for the pushforward density:

$$q_{\theta}(g_{\theta}(z)) = (g_{\theta}|_{\mu})(g_{\theta}(z)) = \mu(z) \left|(\mathrm{d}g_{\theta})_z\right|^{-1}, \quad (3)$$

where $\left|(\mathrm{d}g_{\theta})_z\right|$ represents the determinant of the Jacobian of g_{θ} evaluated at the point z. This finally allows us to rewrite Eq. (1) in the following explicit form, after performing some simplifications:

$$-\max_{\theta} \inf_{\phi} \mathbb{E}_{\hat{x} \sim p} \log \frac{\mu(\hat{z})}{|(\mathrm{d}g_{\theta})_{\hat{z}}|} + \frac{\mu(\hat{z})}{|(\mathrm{d}g_{\theta})_{\hat{z}}|\nu_{\phi}(\hat{x})} + \mathbb{E}_{z \sim \mu} \log \frac{\mu(z)}{|(\mathrm{d}g_{\theta})_z|\nu_{\phi}(g_{\theta}(z))}. \quad (4)$$

2.2 VARIATIONAL INTERPRETATION

Equation (1) can be derived via a variational lower bound derived from Fenchel conjugacy, using a technique similar to [28, 29]. Our approach of pairing this convex conjugate with the pushforward direct density estimation motivates our method's name: Convex Conjugate Coupled Pushforward Optimization (C3PO). Observe that the Jeffrey divergence can be written as $\min_q -\mathbb{E}_{\hat{x} \sim p} \log q(\hat{x}) + \mathbb{E}_{x \sim q} \log q(x) - \mathbb{E}_{x \sim q} \log p(x)$. Since q can be sampled, evaluated, and differentiated (Sec. 2.1), but p can only be sampled, our goal in this section is to convert $-\mathbb{E}_{x \sim q} \log p(x)$ to something expressable in terms of expectations wrt. p and q. This is achieved by applying the Fenchel-Young inequality to the function $f(p) := -\log p$, which yields $-\log p \geq \sup_{\lambda < 0} \lambda p - (-1 - \log(-\lambda))$. Substituting this inequality in place of $-\log p(x)$ yields the following lower bound of $-\mathbb{E}_{x \sim q} \log p(x)$:

$$\int_X q(x)(\sup_{\lambda < 0} \lambda p(x) + \log(-\lambda) + 1)\, \mathrm{d}x = 1 + \sup_{\lambda < 0} \int_X q(x)\left(\lambda(x)p(x) + \log(-\lambda(x))\right)\, \mathrm{d}x, \quad (5)$$

where the sup on the right-hand side is taken over all functions $\lambda : X \to \mathbb{R}^-$ mapping the domain to a negative scalar. Observing that $\int q(x)\lambda(x)p(x)\, \mathrm{d}x$ can be written either as $\mathbb{E}_{x \sim q} \lambda(x)p(x)$ or $\mathbb{E}_{\hat{x} \sim p} \lambda(\hat{x})q(\hat{x})$, and making the substitution $\nu = -1/\lambda$, we have the equivalent bound

$$-\mathbb{E}_{x \sim q} \log p(x) \geq 1 + \sup_{\nu > 0} \mathbb{E}_{\hat{x} \sim p} - \frac{q(\hat{x})}{\nu(\hat{x})} - \mathbb{E}_{x \sim q} \log \nu(x). \quad (6)$$

Substituting this the Jeffrey divergence yields Eq. (1).

2.3 INTERPRETATION AS LEARNING A GIBBS DISTRIBUTION

Although we have so far viewed our goal as primarily learning q, we now observe that our method can also be interpreted primarily as a way of learning ν as a Gibbs distribution approximating p. Learning a Gibbs distribution, or a more general *energy-based model* [22], is a very general and effective way to impose strong domain-specific regularization on probability distributions over high-dimensional data. Generally, this is achieved by structuring the energy function $V_\phi := \log \nu_\phi$ to assign similar energies to similar examples; for example, a convolutional neural network might constitute a good energy for image generation, since the structure of a CNN encodes some degree of translational invariance. Unfortunately, inference and learning with high-dimensional Gibbs distributions is difficult.

Our method can be viewed as a way to train a Gibbs distribution that circumvents some of these difficulties. In this view, the inner optimization in Eq. (1) is interpreted as minimizing a weighted divergence between p and ν; the weights are exactly q. Specifically, we observe that the inner optimization in Eq. (1) minimizes the following weighted Itakura-Saito divergence [18, 10]:

$$\min_\phi \int q(x) \left(\frac{p(x)}{\nu_\phi(x)} - \log \frac{p(x)}{\nu_\phi(x)} - 1 \right) \mathrm{d}x \quad (7)$$

It would seem reasonable to choose the weights q as $q = p$; since p cannot be evaluated directly, alternating optimization is a sensible alternative. Minimizing Eq. (7) intuitively gives us the best Gibbs approximation of p over the support of q. Fig. 2 illustrates why choosing a structured Gibbs parameterization of ν helps reduce overfitting in q as well as ν. When we fit ν via (7) (left part of figure), correlations built into the energy function ensure that pushing up the energies of observed data also pushes up the energies of unobserved data. When we then fix ν and optimize Eq. (1) in q (right part of figure), high energies assigned to the unobserved data prevent pruning the unobserved data from the support of q, while appropriately pruning low-energy modes of q.

3 EXPERIMENTS

We conducted experiments on four datasets of vehicle trajectories, where the objective is to forecast a distribution over the vehicle's future locations $x \in \mathbb{R}^{20 \times 2}$ given contextual information about each scene. The contextual information includes 2 seconds of the vehicle's previous position, as well as a Bird's Eye View (BEV) map of visual scene features. Our experiments are designed to quantify two key aspects of generative modeling: the learned model's likelihood of held-out test data (*i.e.* the negative forward cross-entropy $-H(p, q)$), and the quality of samples from the learned model (*i.e.*

Figure 2: Illustration of why using a structured Gibbs representation for ν helps prevent overfitting of ν and q. Green contours (left two figures) depict support of ν; blue contours depict support of q.

Figure 3: Comparison of methods on a test scene from the BEVWORLD1K dataset. Left column: The input BEV map (roads in black), accompanied by 100 demonstrations of possible behavior (in blue). Each method is visualized with 60 of each samples. For the methods that learn a cost map, the learned cost map is blended with the input BEV feature map.

the negative reverse cross-entropy $-H(q, p)$). Our hypotheses are: *1)* C3PO *will achieve superior sample-quality performance to other methods 2)* C3PO *will learn a high-quality q, partially due to its ability to perform direct density evaluation and optimization of q 3)* C3PO *will learn an interpretable ν that penalizes bad samples.*

Two of the four datasets are synthetic (BEVWORLD 1 and BEVWORLD1K), with known roads, enabling us to construct samples from a reasonable p distribution, approximate p via KDE, and measure the reverse cross-entropy $H(q, p_{\text{KDE}})$. We also calculate the percentage of trajectory points on the road as another measure of sample quality. Details of how we generate BEVWORLD are in the supplement. We also experiment with two real-world datasets: the KITTI dataset, and the CALIFORECASTING dataset [34].

3.1 IMPLEMENTATION AND BASELINES

Given our setting is that of forecasting future vehicle trajectories, we leverage ideas from Inverse Reinforcement Learning [27, 47, 45], to structure our Gibbs energy V as a spatial *cost map*: where

Table 1: Comparison of methods in two datasets. Left: Single BEVWorld Scene (identical train and test), 300 experts, 1800 policy samples. Right: BEVWorld 100 training scenes, 1000 test scenes, 100 experts/scene, 12 policy samples/scene. Means and their standard errors are reported. Bold indicates the best performing method among methods with nondegenerate $-H(p, q)$ (*i.e.* fGAN Jeffrey is degenerate). CVAE's $-H(p, q)$ is estimated via MC sampling 300 times per scene, see [41].

	BEVWORLD 1			BEVWORLD1K		
Method	$-H(p, q)$	$-H(q, p_{\text{KDE}})$	Road %	$-H(p, q)$	$-H(q, p_{\text{KDE}})$	Road %
R2P2	$\mathbf{83.7} \pm 0.2$	-46.6 ± 0.5	0.988	$\mathbf{96.0} \pm 0.03$	-61.6 ± 0.6	0.922
C3PO (ours)	82.6 ± 0.3	$\mathbf{-44.8} \pm 0.4$	$\mathbf{1.000}$	92.7 ± 0.1	$\mathbf{-48.7} \pm 0.3$	$\mathbf{0.989}$
R2P2 GAIL	64.6 ± 2.0	-55.6 ± 1.0	0.952	62.0 ± 0.6	-74.6 ± 0.8	0.886
CVAE*	18.6 ± 3.7	-45.3 ± 1.7	0.990	12.5 ± 0.3	-71.3 ± 0.8	0.865
fGAN KL	16.6 ± 0.6	-294.4 ± 22	0.568	18.6 ± 0.03	-303 ± 2.6	0.698
fGAN Reverse KL	-17.3 ± 2.9	-171 ± 8.5	0.706	-11.6 ± 0.2	-235 ± 1.8	0.709
fGAN Jeffrey	$-7e4 \pm 6e3$	-42.0 ± 0.05	1.000	$-5e3 \pm 39$	-46.1 ± 0.08	0.970

Table 2: Comparison of methods in two real-world datasets: KITTI and CALIFORECASTING. Means and their standard errors are reported. Bold indicates the best performing method among methods with nondegenerate $-H(p, q)$ (*i.e.* fGAN Jeffrey is degenerate).

Method	KITTI		CALIFORECASTING	
	$-H(p, q)$	$V_\phi^{\text{KITTI}}(q)$	$-H(p, q)$	$V_\phi^{\text{CALIF}}(q)$
R2P2	$\mathbf{63}.7 \pm 0.8$	-744 ± 20	$\mathbf{74.1} \pm 0.38$	-6.50 ± 3.9
C3PO (ours)	61.5 ± 0.7	$-\mathbf{457} \pm 13$	73.5 ± 0.4	$\mathbf{57.3} \pm 1.4$
R2P2 GAIL	54.9 ± 0.7	-693 ± 17	46.9 ± 0.3	-61.1 ± 6.1
CVAE*	9.22 ± 0.9	-555 ± 9.9	10.1 ± 0.9	48.3 ± 1.5
fGAN KL	32.9 ± 1.3	-693 ± 10	9.55 ± 0.02	-568 ± 20
fGAN Reverse KL	12.8 ± 0.08	-1362 ± 33	-89.7 ± 3.1	21.8 ± 2.6
fGAN Jeffrey	$-2e4 \pm 2e3$	-195 ± 4.0	$-2e4 \pm 7e2$	69.5 ± 0.1

$\log \nu_\phi = V_\phi(x) = \sum_{t=1}^{T} R_\phi(x_{t0}, x_{t1}; \text{BEV})$, and $R_\phi(a, b; \text{BEV})$ is the output of a CNN that can be interpolated at 2d positions of the form (a, b). This structure enables ν to penalize trajectories that travel to locations it perceives to be bad, *e.g.* locations with obstacles, or locations far from a perceived road. Additionally, in order to mitigate numerical issues of computing q/ν, we mix in a small amount of q into ν: $\nu \leftarrow \alpha q + \nu$, with $\alpha \leq 10^{-4}$. We take care to ensure our optimization treats αq as a constant, although it may not be necessary.

We compare our method, C3PO, to several state-of-the-art approaches in imitation learning and generative modeling: Generative Adversarial Imitation Learning (GAIL) [14], f-GAN [29], the CVAE method of DESIRE [23], and R2P2[34]. In each baseline, we use architectures as similar to our own method as possible: the policy (generator) architecture of GAIL and the generator architecture of f-GAN are identical to the generator architecture of our own approach. The same architecture used for V_ϕ in our method was also used for the discriminators in all baselines.

Our implementation of the q architecture is based on R2P2 [35]. One key difference between our method, C3PO, and R2P2, is that R2P2 does not have an adversarial component; its main focus is learning the forward KL term, the first component of C3PO's objective function. R2P2 starts from a similar objective: the symmetric sum of cross-entropies. However, it relies on a cruder approximation of $H(q, p)$, because it learns an approximating $\tilde{p}$ for $H(q, \tilde{p})$ offline, with no interaction from q.

3.2 SYNTHETIC EXPERIMENTS

BEVWORLD 1contains a single scene with 300 samples from p. This setting is *unconditional*: the contextual information provided is identical, and not directly useful for modeling p. This setting also provides a fairer comparison to fGAN methods, which left the extension of fGAN to contextual settings as future work [29]. Table 1 shows the results of BEVWORLD 1 experiments. We observe that R2P2 and C3PO achieve the best $-H(p, q)$ scores, with C3PO outperforming all nondegenerate methods in its sample quality. This evidence supports hypotheses 1) and 2): C3PO achieves superior sample quality and high-quality data density. We also observed C3PO to be very stable throughout training in terms of $H(p, q)$: it was as easy to train it as R2P2 in all experiments.

We also observe that while fGAN KL indirectly learns a q with some support for p, its samples are quite poor. This matches expectations, as the forward KL divergence fails to impose much penalty on sample quality [16]. fGAN Jeffrey is the fGAN method most similar to our approach because it uses the Jeffrey divergence. We observe it to suffer mode collapse in all of our experiments, a similar result to [29], in which fGAN Jeffrey had the worse test-set likelihood.

Next, we consider BEVWORLD1K, in which 100 training scenes, each with 100 samples from p, are used to learn *conditional* generative models. There are 1000 scenes in the test set. Table 1 shows the result of these experiments. We observe results similar to BEVWORLD1K, again supporting hypotheses 1) and 2). C3PO can learn in the conditional setting to produce high-quality samples from a distribution with good support of p. We display example results in Fig. 3, and observe several methods, including C3PO , learn a cost-map representation that penalizes samples not on the road. This evidence of the learned intuitive perceptual measurement of ν supports hypothesis 3).

Figure 4: **Left:** Comparison of methods under the learned $V_\phi^{\text{KITTI}}(q)$ criterion. Each row corresponds to a method, and each column corresponds to the method's result on the item at a specific level of performance, from worst (left) to best (right) of results on 100 scenes. Each image is composed of the learned $V_\phi^{\text{KITTI}}(q)$ blended with the input BEV features, sample trajectories from each method (red), and the true future (blue). The learned V often penalizes samples that go off of the road or into obstacles inferred from the features. C3PO usually produces the best samples under this metric. **Right:** Evaluation of sample quality on test data from the KITTI dataset (a) and CALIFORECASTING dataset (b). Each approach generated 12 trajectory samples per scene, and the mean V_ϕ score was calculated for each scene. The results are displayed as a normalized cumulative histogram, where the y-value at x is the percentage of scenes that received $V \le x$. At almost every given V, C3PO is likelier to have more samples above the given V than other methods.

Figure 5: Comparison of methods on a set of random scenes from the CALIFORECASTING test set. Scene indices were selected uniformly at random (once) from the possible test indices. Each image shows the learned $V_\phi^{\text{CALIF}}(q)$ blended with the input BEV features, 12 sample trajectories from each method (red), and the true future (blue). V learns to penalize samples that go off of the road or into obstacles.

3.3 REAL-WORLD EXPERIMENTS

We now experiment with real-world data, in which each method is provided with noisy contextual information, and is evaluated by its ability to produce a generative model and high-quality samples. Evaluation of sample quality is more difficult in this scenario: we have only one sample of p in each scene, precluding construction of p_{KDE}, and there are no labels of physical roads, precluding computation of on-road statistics. Fortunately, evaluation of $-H(p, q)$ is still possible.

After observing the learned V_ϕ of C3PO on both synthetic and real data, we found V_ϕ to be generally interpretable and intuitively good: it assigns low cost to roads it learns to perceive and it assigns high cost to obstacles it learns to perceive. We therefore employed our learned model V_ϕ to quantitatively evaluate samples from all methods. Fig. 4 illustrates results from several approaches visualized with V and point cloud features from the BEV, at various quantiles of each method's performance under V. Fig. 5 (left) illustrates each method on a set of randomly sampled scenes. In both figures, V perceives and assigns penalty to regions around obstacles in the point cloud data. Note that this energy is learned implicitly, because demonstrations from p avoid obstacles. These results provide further support for hypothesis 3).

Quantitative results are shown in Table 2. We find that results are, overall, similar to results on the other datasets. C3PO produces a high-performing q in terms of both its likelihood, $-H(p, q)$, as well as the quality of its samples, V. Additionally, we show evaluation of V for the top methods in Fig. 4 (right). Together, these results further strengthen evidence in support of all of our hypotheses.

4 RELATED WORK

The initial motivation for our work was the apparent dichotomy between sample quality and mode coverage in existing deep generative models; this phenomenon has been noted and quantified in work such as [44, 26, 4, 15, 16]. Our work synthesizes several techniques from prior work to address these issues, including the Fenchel-variational principle from work such as [28, 29], the well-known reparameterization trick [19, 39], and analytic pushforward-based density estimators such as normalizing flows [32, 20], RealNVP [9], and related models [25, 11, 30, 42, 33]. Comparatively little work has explored combining these methods, with some exceptions. Combining a RealNVP [9] density estimator with a GAN objective was considered in [12]; however, this is susceptible to the problems inherent with GANs mentioned in the introduction. A pushforward-based density estimator was employed in conjunction with variational inference to optimize the classical Bayesian evidence lower bound in [20], but this cross-entropy objective suffers from the previously-mentioned problems with optimizing $KL(p \parallel q)$ alone, as do all methods based on this objective, including [9, 11, 30, 42].

Our work is also comparable to the extensive literature on learning deep graphical models, including variants of Boltzmann machines [1, 38] and various proposals for learning deep CRFs and structured energy-based models [22] based on inference techniques including convex optimization [31, 8, 2, 40], various forms of unrolled inference [36, 46, 43], pseudolikelihood [24], and continuous relaxation [5], among other techniques [15]. Viewed as a way to learn a deep graphical model, the most important distinguishing factor of our work is the fact that our method does not need to perform inference directly, as discussed in Sec. (2.3). To the extent that q is viewed as (indirectly) performing inference, our method and other deep generative models bears some similarity to the wake-sleep algorithm, which also alternates between optimizing a model distribution and an "inference" distribution using complementary divergences [15]. Score-matching [17] also learns a Gibbs distribution without inference; however, unlike our method, score-matching does not learn an inference distribution.

5 CONCLUSION

We have demonstrated how GANs may be effectively regularized by reparameterizing the discriminator to be a function of the model density and a structured Gibbs density, showing how this may be achieved by optimizing a Jeffrey divergence loss, assuming the generator is invertible, and applying a variational bound based on Fenchel conjugacy. Applied to a trajectory forecasting problem, we observed superior mode coverage and qualitative results compared to traditional GANs. We hope to soon demonstrate the general applicability of our approach by applying it to the task of image generation as well.

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